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Vacancy–interstitial interactions in crystalline Silicon MATTHEW J. BECK, L. TSETSERIS, S.T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, Nashville, TN — Extensive experimental and theoretical investigations of fundamental defects in Si have led to the conclusion that both interstitials and vacancies diffuse athermally according to a carrier recombination-enhanced Bourgoin-Corbett mechanism. It is therefore widely accepted that Si vacancy-interstitial pairs, or Frenkel pairs (FPs), either rapidly recombine or dissociate, even at cryogenic temperatures. This has recently been challenged by X-ray scattering experiments that are interpreted to show FPs in Si persisting to > 100 K (Partyka, P., et al., *Phys. Rev. B* v. 64 art. no. 235207). Here we report first-principles density functional theory calculations of the properties of FPs in Si. A novel electronic interaction involving charge transfer from the interstitial to the vacancy in a FP is described. In a bound FP, this interaction suppresses the athermal diffusion mechanisms of both the interstitial and vacancy. This reconciles the existing experimental results by establishing that there are thermal barriers to the recombination or dissociation of bound FPs, but not affecting the previously described athermal diffusion of isolated interstitials and vacancies. This work supported by the AFOSR-MURI program.

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